

## CHEMICAL PHYSICS

Volume 127, number 1,2,3, 15 November 1988

### CONTENTS

Polarizabilities and local fields in a diacetylene monomer and polymer crystal M. Hurst and R.W. Munn	1
Calculation of the Bloch effective Hamiltonian as an expectation value F.X. Gadea and J.-L. Heully	9
Theoretical analysis of Franck-Condon and vibronic activity of the $a_g$ and $b_{3g}$ modes in the $S_0 \leftrightarrow S_1$ transitions in anthracene F. Zerbetto and M.Z. Zgierski	17
A new perturbative approach of the resonance eigenvalue problem in high parameterized systems G. Jolicard and J. Humbert	31
How to obtain a mixed local-non-local molecular wavefunction P. Karafiloglou and P. Akrivos	41
Ab initio quantum chemical study of the $S_N2$ reaction, $CH_3F + H^- \rightarrow CH_4 + F^-$ , in the gas phase Z. Havlas, A. Merkel, J. Kalcher, R. Janoschek and R. Zahradník	53
The nature of the SCF basis set superposition error. Application of the indirect counterpoise method in polyatomic van der Waals molecules S. Tolosa, J.J. Esperilla, J. Espinosa and F.J. Olivares del Valle	65
Dissociation dynamics of $FC(O)O$ and $CIC(O)O$ radicals J.S. Francisco and A.N. Goldstein	73
Classical differential cross sections and rainbows for a system of arbitrary dimensionality T.C.M. Horn, A.W. Kleyn and E.A. Gislason	81
Collision lifetime matrix analysis of the two lowest energy resonances in the collinear $H + H_2$ system J.A. Kaye and A. Kuppermann	97
Semiclassical model for energy transfer in polyatomic molecules. XIII. Biomolecules G.D. Billing	107
Theory of magnetic vibrational circular dichroism spectra in molecules of cubic symmetry M. Pawlikowski	121
Intramolecular motion in the tert-butyl radical as studied by muon spin rotation and level-crossing spectroscopy P.W. Percival, J.-C. Brodovitch, S.-K. Leung, D. Yu, R.F. Kiefl, G.M. Luke, K. Venkateswaran and S.F.J. Cox	137
A planar rotor model for cholestan spin label motion in phospholipid multibilayers with high order A.J. Dammers, Y.K. Levine, K. Balasubramanian and A.H. Beth	149
Two-color multiphoton dissociation/ionization of jet-cooled $Cr^{III}(acac)_3$ and $Cr^0(CO)_6$ . Appearance energies of Cr atom N. Mikami, R. Ohki and H. Kido	161

*(continued on page 3 of cover)*

## CONTENTS

(continued from page 4 of cover)

High-resolution spectroscopy of highly excited electronic states by pulsed-cw double resonance in a molecular beam. A study of the NO(E-A) system G. Meijer, M. Ebben and J.J. ter Meulen	173
Supersonic jet spectroscopy of S <sub>2</sub> O D.J. Clouthier and M.L. Rutherford	189
Picosecond infrared multiphoton ionization of chromyl chloride Y.J. Xie, C.C. Chin, M. Cecere and H.S. Kwok	197
Radiative lifetimes, diffusion and energy pooling of Sr(5s5p( <sup>3</sup> P <sub>J</sub> )) and Sr(5s4d( <sup>1</sup> D <sub>2</sub> )) studied by time-resolved atomic emission following pulsed dye-laser excitation D. Husain and G. Roberts	203
The energy pooling reactions between Cd(5 <sup>3</sup> P <sub>J</sub> ) atoms H. Umemoto, J. Kikuma, A. Masaki and S. Sato	227
Mechanisms of the strongly exothermic charge separation reaction in the excited singlet state. Picosecond laser photolysis studies on aromatic hydrocarbon-tetracyanoethylene and aromatic hydrocarbon-pyromellitic dianhydride systems in polar solutions N. Mataga, Y. Kanda, T. Asahi, H. Miyasaka, T. Okada and T. Kakitani	239
The bell-shaped energy gap dependence of the charge recombination reaction of geminate radical ion pairs produced by fluorescence quenching reaction in acetonitrile solution N. Mataga, T. Asahi, Y. Kanda, T. Okada and T. Kakitani	249
Electronic and vibrational relaxation of CO in Ar and Kr matrices J. Bahrdt and N. Schwentner	263
Magnetic field effects on positronium in liquids I. Billard, J.-Ch. Abbé and G. Duplâtre	273
A neutron diffraction and RISM study of liquid Fe(CO) <sub>5</sub> at 295 K J.B. van Tricht and J.S. Sjoerdsma	279
Influence of the assumed molecule environment on the value of calculated dipole moment J.J. Makosz and K. Peika	287
An optically detected magnetic resonance study of Mn <sup>4+</sup> in Cs <sub>2</sub> GeF <sub>6</sub> and K <sub>2</sub> GeF <sub>6</sub> E. Lifshitz and A.H. Francis	297
ESR studies of metallocene intercalated Cd <sub>2</sub> P <sub>2</sub> S <sub>6</sub> E. Lifshitz, D.A. Cleary and A.H. Francis	305
Electronic states and potential energy surfaces of gold and silver trimer K. Balasubramanian and M.Z. Liao	313
Electron transfer accompanied by bond rupture D.V. Matyushov and Y.A. Maletin	325
<sup>14</sup> N nuclear quadrupole coupling in amides: ab initio studies of formamide and acetamide and a comparison with microwave and NQR data M.H. Palmer	335

(continued on previous page)

## CONTENTS

(continued from page 3 of cover)

A proposal for avoiding overestimation in the counterpoise basis set superposition error. Application to diatomic van der Waals systems F.J. Olivares del Valle, S. Tolosa, E.A. Ojalvo and J. Espinosa	343
The linear mixture rule in chemical kinetics. II. Thermal dissociation of diatomic molecules C. Carruthers and H. Teitelbaum	351
Dispersion and polarization forces associated with the ion-pair states of diatomic molecules K. Lawley	363
Molecular dynamics simulation of conformational transitions and solvatochromism of polydiacetylenes G.A. Vinogradov, M.M. El'yashevich and A.A. Ovchinnikov	373
Direct observation, by the matrix isolation technique, of nitric oxide effects in low-pressure silane discharges L. Abouaf-Marguin, A. Lloret, M. Oria and B. Seoudi	385
VUV laser spectroscopy of $\text{Xe}_2$ in the $\text{C}' 1_u$ state K. Tsukiyama, M. Tsukakoshi and T. Kasuya	393
Scalar and vector properties of $\text{RO}(\text{A}^2\Sigma^+)$ formed in the VUV photodissociation of $\text{R}_2\text{O}_2$ ( $\text{R}=\text{H, D}$ ) K.-H. Gericke, H. Gölzenleuchter and F.J. Comes	399
X-ray photoelectron spectra of polycarbazole, carbazole and polypyrene: analysis of the origin of peak asymmetry observed in their C 1s spectra S. Hino, M. Nakazato and K. Matsumoto	411
keV collisions of $[\text{H}_3]^+$ and isotopomer ions J. Bordas-Nagy and J.L. Holmes	419
The dissociative electroionization of ammonia and ammonia- $d_3$ . III. The $\text{N}^+$ dissociation channel. General conclusions about the dissociation of $\text{NH}_3^+$ R. Locht and J. Momigny	435
The effect of recoil on the inelastic neutron scattering spectra of molecular vibrations J. Tomkinson	445
A study of carrier generation mechanism in benzimidazole perylene/tetraphenyldiamine thin film structures Z.D. Popovic, A.-M. Hor and R.O. Loutfy	451
Author index	458
List of subjects	462
Subject index	464
Instructions to authors	477